



Physical Properties for Lipids Based Process and Product Design

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At-A-Glance

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Lipid processing covers several oil and fats technologies such as: edible oil production, biodiesel production, oleochemicals (e.g.: food additives, detergents) and pharmaceutical product manufacturing. New demands regarding design and development of better products and more sustainable processes related to lipids technology, emerge according to consumers demanding improved product manufacturing from sustainable resources and new legislation regarding environmental safety [1]. Physical and thermodynamic property data and models for prediction of pure compound properties and mixtures properties involving lipids represent the basic and most important requirements for process-product design, simulation and optimization. Experimentally measured values of involved compounds are desirable, but in most of the cases these are not available for all the compounds and properties needed. The lack of properties is even larger for mixtures properties. Therefore there is a highly need of predictive properties models.

Oleochemical industry, along with all other lipids processing technologies, presents many challenges in relation to thermodynamic and physical properties as a result of lack of experimental data for pure compounds and their mixtures. Due to these gaps, lipids involved industries are not able to exploit all the advances achieved within computer aided methods and tools, for which property data and models represent the basic requirements to perform process design, simulation and optimization, as well as product design. Another challenge comes from the availability of the data and models within commercial available software [2].

Recent developments within lipid property modelling, as well as new physical and thermodynamic data availability, allowed the development of our in-house SPEED Lipids Database. The database is directly connected with external computer aided tools, such as PROII and ICAS suite, and it is organised within two parts: one is dedicated to the pure compounds and their properties, while the other is dedicated to the mixtures phase equilibria. In product-process design, the chemicals database together with the lipids database is used.

For the development of the database – pure compound part, available data for lipids in terms of their molecular description and a range of properties were collected in special attention to the needs for model-based design and analysis within oleochemical industry. Available experimental data was collected for the identified lipids and their corresponding properties. The database contains 330 pure compounds organised within 18 categories (e.g.: fatty acids, triacylglycerides, diacylglycerides, monoacylglycerides, methyl esters, ethyl esters, isopropyl esters, carotenoids, triterpenealcohols, phospholipids, fatty alcohols, sterols, vitamin E, etc.). The experimental data was collected for 7 primary properties (e.g.: critical temperature, pressure and volume, Gibbs free energy of formation, enthalpy of formation, melting point, and normal boiling point), and 6 temperature dependent properties (vapour pressure, liquid heat capacity, liquid density, liquid thermal conductivity, viscosity, and surface tension). To fill in the gaps within the database models for 14 primary properties (e.g.: molecular weight, critical properties, melting point, normal boiling point, enthalpy of formation, enthalpy of fusion, Gibbs free enthalpy of formation, dipole moment, acentric factor, specific gravity, dipole moment, liquid volume) and 10 temperature dependent properties (e.g.: vapour pressure, liquid enthalpy, liquid viscosity, liquid thermal conductivity, ideal

enthalpy, surface tension, latent heat, liquid density, vapour density, vapour thermal conductivity) were implemented. The chemicals database contains 45500 chemicals and more than 27 different properties.

The mixture phase equilibria component of the lipids database contains a collection of over 4500 measured data point corresponding 332 different phase equilibria data sets (92 VLE, 91 LLE, 70 SLE and 79 solubility data) for binary and multi component mixtures. Consistency test were performed for all the VLE and SLE data sets available in the database. From the available VLE data sets, original UNIFAC parameters were regressed, allowing better representation and prediction of the phase equilibria.

The following features are available within SPEED Lipids database: property data consistency test; optimization based data regression to estimate the model parameters; knowledge representation and search engine for database use knowledge representation and search engine for database; computer aided modelling tool to quickly and efficiently develop the necessary property prediction models. Also, a systematic work flow for database maintenance and development is provided. All databases are integrated with process and product simulators. The presentation will highlight the use of the database and property models in case studies involving process-product design.

Reference

[1] Diaz-Tovar C, Mustafa A., Hukkerikar, A., Quaglia A, Sin G, Kontogeorgis G, Sarup B, Gani R. Lipid Processing Technology: Building a Multilevel Modeling Network. In: Pistikopoulos E. N., Georgiadis M. C., Kokossis A, editors. Proceedings of the 21st European Symposium on Computer Aided Process Engineering 2011, 29:256–260.

[2] Sarup B. Advances and Challenges in Modelling of Processing of Lipids. In: Gernaey K. V., Huusom J. K., Gani R., editors. Proceedings of the 25th European Symposium on Computer Aided Process Engineering 2015, 37:117-122.

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